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Hamiltonization of Nonholonomic Systems and the Inverse Problem of the Calculus of Variations

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Abstract

We introduce a method which allows one to recover the equations of motion of a class of nonholonomic systems by finding instead an unconstrained Hamiltonian system on the full phase space, and to restrict the resulting canonical equations to an appropriate submanifold of phase space. We focus first on the Lagrangian picture of the method and deduce the corresponding Hamiltonian from the Legendre transformation. We illustrate the method with several examples and we discuss its relationship to the Pontryagin maximum principle.

Keywords: nonholonomic system, inverse problem, Pontryagin's principle, control system, Hamiltonian, quantization.

1 Introduction

The direct motivation of this paper lies with some interesting results that appeared in the paper [17], wherein the authors propose a way to quantize some of the well-known classical examples of nonholonomic systems. On the way to quantization, the authors propose an alternative Hamiltonian representation of nonholonomic mechanics. In short, the authors start off from the actual solutions of the nonholonomic system, and apply a sort of Hamilton-Jacobi theory to arrive at a Hamiltonian whose Hamilton's equations, when restricted to a certain subset of phase space, reproduce the nonholonomic dynamics. Needless to say, even without an explicit expression for the solutions one can still derive a lot of the interesting geometric features and of the qualitative behaviour of a nonholonomic system. However, the "Hamiltonization" method introduced in [17] is not generalized to systems for which the explicit solution is not readily available, and hence cannot be applied to those systems.

In this paper, we wish to describe a method to Hamiltonize a class of nonholonomic systems that does not depend on the knowledge of the solutions of the system. Instead, we will start from the Lagrangian equations of motion of the system and treat the search for a Hamiltonian which

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Hamiltonizes the dynamics as the search for a regular Lagrangian. That is, we will explain how one can associate to the nonholonomic equations of motion a family of systems of second-order ordinary differential equations and we will apply the inverse problem of the calculus of variations [12, 27] on those associated systems. If an unconstrained (or free) regular Lagrangian exists for one of the associated systems, we can always find an associated Hamiltonian by means of the Legendre transformation. Since our method only makes use of the equations of motion of the system, it depends only on the Lagrangian and constraints of the nonholonomic system, but not on the knowledge of the exact solutions of the system.

A system for which no exact solutions are known can only be integrated by means of numerical methods. In addition to the above mentioned application to quantization, our Hamiltonization method may also be useful from this point of view. A geometric integrator of a Lagrangian system uses a discrete Lagrangian that resembles as close as possible the continuous Lagrangian (see e.g. [23]). On the other hand, the succes of a nonholomic integrator (see e.g. [9, 15]) relies not only on the choice of a discrete Lagrangian but also on the choice of a discrete version of the constraint manifold. It seems therefore reasonable that if a free Lagrangian for the nonholonomic system exists, the Lagrangian integrator may perform better than a nonholonomic integrator with badly chosen discrete constraints. Work along these lines is in progress.

It should be remarked from the outset that the Hamiltonization we have in mind is different from the "Hamiltonization" used in e.g. the papers [5, 14]. Roughly speaking, these authors first project a given nonholonomic system with symmetry to a system on a reduced space and then use a sort of time reparametrization to rewrite the reduced system in a Hamiltonian form in the new time (this is the so-called Chaplygin's reducibility trick). In contrast, we embed the (unreduced) nonholonomic system in a larger Hamiltonian one.

In the second part of the paper, we show that in the cases where a regular Lagrangian (and thus a Hamiltonian) exists, we can also associate a first order controlled system to the nonholonomic system. As an interesting byproduct of the method it turns out that if one considers the optimal control problem of minimizing the controls for an appropriate cost function under the constraint of that associated first order controlled system, Pontryagin's maximum principle leads in a straightforward way to the associated Hamiltonians.

We begin with a quick review of nonholonomic mechanics in section 2, where we introduce some of the well-known classical nonholonomic systems which fall into the class of systems we will be studying in the current paper. We then begin our investigations in section 3 with the Lagrangian approach to the problem. We detail the various ways to associate a second-order system to a nonholonomic system, which then forms the backbone of our subsequent analysis. In section 4 we briefly review the set up for the inverse problem of the calculus of variations, and then apply it to some of the associated second-order systems. We derive the corresponding Hamiltonians in section 5 and discuss their relation with Pontryagin's maximum principle in section 6. At the end of the paper we provide a few directions for future work on generalizing our findings to more general nonholonomic systems, as well as applying them to quantize nonholonomic systems.

2 Nonholonomic systems

Nonholonomic mechanics takes place on a configuration space Q with a nonintegrable distribution $\mathcal{D}$ that describes the (linear supposed) kinematic constraints of interest. These constraints are often given in terms of independent one-forms, whose vanishing in turn describes the distribution. Moreover, one typically assumes that one can find a fibre bundle and an Ehresmann connection A on that bundle such that $\mathcal{D}$ is given by the horizontal subbundle associated with A. Such an approach is taken, for example, in some recent books on nonholonomic systems [3, 7].

Let Q be coordinatized by coordinates (r^I, s^α), chosen in such a way that the projection of the above mentioned bundle structure is locally simply $(r,s) \mapsto r$. Moreover, let $\{\omega^\alpha\}$ be a set of independent one-forms whose vanishing describes the constraints on the system. Locally, we can write them as

$$\omega^\alpha(r,s) = ds^\alpha + A^\alpha_I(r,s)dr^I.$$

The distribution $\mathcal{D}$ is then given by

$$\mathcal{D} = \mathrm{span}\{\partial_{r^I} - A^\alpha_I \partial_{s^\alpha}\}.$$

One then derives the equations of motion using the Lagrange-d'Alembert principle, which takes into account the need for reaction forces that enforce the constraints throughout the motion of the system (see e.g. [3]). If $L(r^\alpha, s^a, \dot{r}^\alpha, \dot{s}^\alpha)$ is the Lagrangian of the system, these equations are

$$\frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{r}^I}\Big) - \frac{\partial L}{\partial r^I} = \lambda_\alpha A^\alpha_I \quad \text{and} \quad \frac{d}{dt}\Big(\frac{\partial L}{\partial \dot{s}^\alpha}\Big) - \frac{\partial L}{\partial s^\alpha} = \lambda_\alpha,$$

together with the constraints $\dot{s}^\alpha = -A^\alpha_I \dot{r}^I$. One can easily eliminate the Lagrange multipliers λ and rewrite the above equations in terms of the constrained Lagrangian

$$L_c(r^I, s^\alpha, \dot{r}^I) = L(r^I, s^\alpha, \dot{r}^I, -A^\alpha_I \dot{r}^I).$$

The equations of motion, now in terms of L_c, become

$$\left\{\begin{array}{rcl} \dot{s}^\alpha &=& -A^\alpha_I \dot{r}^I, \\ \dfrac{d}{dt}\Big(\dfrac{\partial L_c}{\partial \dot{r}^I}\Big) &=& \dfrac{\partial L_c}{\partial r^I} - A^\alpha_I \dfrac{\partial L_c}{\partial s^\alpha} - \dot{r}^J B^\alpha_{IJ} \dfrac{\partial L}{\partial \dot{s}^\alpha}. \end{array}\right. , \tag{1}$$

where $B^\alpha_{IJ} = \partial_{r^J} A^\alpha_I - \partial_{r^I} A^\alpha_J + A^\beta_I \partial_{s^\beta} A^\alpha_J - A^\beta_J \partial_{s^\beta} A^\alpha_I$.

To illustrate this formulation, consider perhaps the simplest example: a nonholonomically constrained free particle with unit mass moving in $\mathbb{R}^3$ (more details can be found in [3], [26]). In this example one has a free particle with Lagrangian and constraint given by

$$L = \frac{1}{2}\left(\dot{x}^2 + \dot{y}^2 + \dot{z}^2\right), \qquad \dot{z} + x\dot{y} = 0. \tag{2}$$

We can form the constrained Lagrangian L_c by substituting the constraint into L, and proceed to compute the constrained equations, which take the form

$$\ddot{x} = 0, \quad \ddot{y} = -\frac{x\dot{x}\dot{y}}{1+x^2}, \quad \dot{z} = -x\dot{y}. \tag{3}$$

Another example of interest is the knife edge on a plane. It corresponds physically to a blade with mass m moving in the xy plane at an angle ϕ to the x-axis (see [24]). The Lagrangian and constraints for the system are:

$$L = \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + \frac{1}{2}J\dot{\phi}^2, \qquad \dot{x}\sin(\phi) - \dot{y}\cos(\phi) = 0, \tag{4}$$

from which we obtain the constrained equations:

$$\ddot{\phi} = 0, \qquad \ddot{x} = -\tan(\phi)\dot{\phi}\dot{x}, \qquad \dot{y} = \tan(\phi)\dot{x}.$$

3 Second-order dynamics associated to a class of nonholonomic systems

Recall from the introduction that we wish to investigate how we can associate a free Hamiltonian to a nonholonomic system. One way to do that is to rephrase the question in the Lagrangian formalism and to first investigate whether or not there exists a regular Lagrangian. Then, by means of the Legendre transformation, we can easily generate the sought after Hamiltonian. Rather than abstractly describing the various ways of associating a second-order system to a given nonholonomic system though, we will instead illustrate the method by means of one of the most interesting examples of a nonholonomic system.

3.1 Associated Second-Order Systems for the vertically rolling disk

The vertical rolling disk is a homogeneous disk rolling without slipping on a horizontal plane, with configuration space $Q = \mathbb{R}^2 \times S^1 \times S^1$ and parameterized by the coordinates (x, y, θ, φ), where (x, y) is the position of the center of mass of the disk, θ is the angle that a point fixed on the disk makes with respect to the vertical, and φ is measured from the positive x-axis. The system has the Lagrangian and constraints given by

$$\begin{aligned} L &= \frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + \frac{1}{2}I\dot{\theta}^2 + \frac{1}{2}J\dot{\varphi}^2, \\ \dot{x} &= R\cos(\varphi)\dot{\theta}, \\ \dot{y} &= R\sin(\varphi)\dot{\theta}, \end{aligned} \tag{5}$$

where m is the mass of the disk, R is its radius, and I, J are the moments of inertia about the axis perpendicular to the plane of the disk, and about the axis in the plane of the disk, respectively. The constrained equations of motion are simply:

$$\ddot{\theta} = 0, \quad \ddot{\varphi} = 0, \quad \dot{x} = R\cos(\varphi)\dot{\theta}, \quad \dot{y} = R\sin(\varphi)\dot{\theta}. \tag{6}$$

The solutions of the first two equations are of course

$$\theta(t) = u_\theta t + \theta_0, \qquad \varphi(t) = u_\varphi t + \varphi_0,$$

and in the case where $u_\varphi \neq 0$, we get that the x- and y-solution is of the form

$$\begin{aligned} x(t) &= \left(\frac{u_\theta}{u_\varphi}\right) R\sin(\varphi(t)) + x_0, \\ y(t) &= -\left(\frac{u_\theta}{u_\varphi}\right) R\cos(\varphi(t)) + y_0, \end{aligned} \tag{7}$$

from which we can conclude that the disk follows a circular path. If $u_\varphi = 0$, we simply get the linear solutions

$$x(t) = R\cos(\varphi_0)u_\theta t + x_0, \quad y(t) = R\sin(\varphi_0)u_\theta t + y_0. \tag{8}$$

The situation in (8) corresponds to the case when φ remains constant, i.e. when the disk is rolling along a straight line. For much of what we will discuss in the next sections, we will exclude these type of solutions from our framework for reasons we discuss later.

Having introduced the vertical disk, let us take a closer look at the nonholonomic equations of motion (6). As a system of ordinary differential equations, these equations form a mixed set of coupled first- and second-order equations. It is well-known that these equations are never variational on their own [3, 7], in the sense that we can never find a regular Lagrangian whose (unconstrained) Euler-Lagrange equations are equivalent to the nonholonomic equations of motion (1) (although it may still be possible to find a singular Lagrangian). There are, however, infinitely many systems of second-order equations (only), whose solution set contains the solutions of the nonholonomic equations (1). We shall call these second-order systems *associated second-order systems*, and in the next section will wish to find out whether or not we can find a regular Lagrangian for one of those associated second-order systems. If so, we can use the Legendre transformation to get a full Hamiltonian system on the associated phase space. On the other hand, the Legendre transformation will also map the constraint distribution onto a constraint submanifold in phase space. The nonholonomic solutions, considered as particular solutions of the Hamiltonian system, will then all lie on that submanifold.

There are infinitely many ways to arrive at an associated second-order system for a given nonholonomic system. We shall illustrating three choices below using the vertical rolling disk as an example.

Consider, for example, taking the time derivative of the constraint equations, so that a solution of the nonholonomic system (6) also satisfies the following complete set of second-order differential equations in all variables (θ, φ, x, y):

$$\ddot{\theta} = 0, \quad \ddot{\varphi} = 0, \quad \ddot{x} = -R\sin(\varphi)\dot{\theta}\dot{\varphi}, \quad \ddot{y} = R\cos(\varphi)\dot{\theta}\dot{\varphi}. \tag{9}$$

We shall call this associated second-order system the *first associated second-order system*. Excluding for a moment the case where $u_\varphi = 0$, the solutions of equations (9) can be written as

$$\begin{aligned}
\theta(t) &= u_\theta t + \theta_0 \\
\varphi(t) &= u_\varphi t + \varphi_0 \\
x(t) &= \left(\frac{u_\theta}{u_\varphi}\right) R\sin(\varphi(t)) + u_x t + x_0, \\
y(t) &= -\left(\frac{u_\theta}{u_\varphi}\right) R\cos(\varphi(t)) + u_y t + y_0.
\end{aligned}$$

By restricting the above solution set to those that also satisfy the constraints $\dot{x} = \cos(\varphi)\dot{\theta}$ and $\dot{y} = \sin(\varphi)\dot{\theta}$ (i.e. to those solutions above with $u_x = u_y = 0$), we get back the solutions (7) of the non-holonomic equations (6). A similar reasoning holds for the solutions of the form (8). The question we then wish to answer in the next section is whether the second-order equations (9) are equivalent to the Euler-Lagrange equations of some regular Lagrangian or not.

Now, taking note of the special structure of equations (9), we may use the constraints (6) to eliminate the $\dot{\theta}$ dependency. This yields another plausible choice for an associated system:

$$\ddot{\theta} = 0, \quad \ddot{\varphi} = 0, \quad \ddot{x} = -\frac{\sin(\varphi)}{\cos(\varphi)}\dot{x}\dot{\varphi}, \quad \ddot{y} = \frac{\cos(\varphi)}{\sin(\varphi)}\dot{y}\dot{\varphi}. \tag{10}$$

We shall refer to this choice later as the *second associated second-order system*.

Lastly, we may simply note that, given that on the constraint manifold the relation $\sin(\varphi)\dot{x} - \cos(\varphi)\dot{y} = 0$ is satisfied, we can easily add a multiple of this relation to some of the equations above. One way of doing so leads to the system

$$\begin{aligned}
J\ddot{\varphi} &= -mR(\sin(\varphi)\dot{x} - \cos(\varphi)\dot{y})\dot{\theta}, \\
(I + mR^2)\ddot{\theta} &= mR(\sin(\varphi)\dot{x} - \cos(\varphi)\dot{y})\dot{\varphi}, \\
(I + mR^2)\ddot{x} &= -R(I + mR^2)\sin(\varphi)\dot{\theta}\dot{\varphi} + mR^2\cos(\varphi)(\sin(\varphi)\dot{x} - \cos(\varphi)\dot{y})\dot{\varphi}, \\
(I + mR^2)\ddot{y} &= R(I + mR^2)\cos(\varphi)\dot{\theta}\dot{\varphi} + mR^2\sin(\varphi)(\sin(\varphi)\dot{x} - \cos(\varphi)\dot{y})\dot{\varphi}.
\end{aligned} \tag{11}$$

For later discussion we shall refer to it as the *third associated second-order system*. We mention this particular second-order system here because it has been shown in [16] (using techniques that are different than those we will apply in this paper) that this complicated looking system is indeed variational! The Euler-Lagrange equations for the regular Lagrangian

$$L = -\frac{1}{2}m(\dot{x}^2 + \dot{y}^2) + \frac{1}{2}I\dot{\theta}^2 + \frac{1}{2}J\dot{\varphi}^2 + mR\dot{\theta}(\cos(\varphi)\dot{x} + \sin(\varphi)\dot{y}), \tag{12}$$

are indeed equivalent to equations (11), and, when restricted to the constraint distribution, its solutions are exactly those of the nonholonomic equations (6). We shall have more to say about this system in section 4.4 below.

3.2 Associated Second-Order Systems in General

We will, of course, not only be interested in the vertically rolling disk. It should be clear by now that there is no systematic way to catalogue the second-order systems that are associated to a nonholonomic system. If no regular Lagrangian exists for one associated system, it may still exist for one of the infinitely many other associated systems. For many nonholonomic systems, the search for a Lagrangian may therefore remain inconclusive. On the other hand, also the solution of the inverse problem of any given associated second-order system is too hard and too technical to tackle in the full generality of the set-up of the section 2. Instead, we aim here to concisely formulate our results for a well-chosen class of nonholonomic systems which include the aforementioned examples and for only a few choices of associated second-order systems.

To be more precise, let us assume from now on that the configuration space Q is locally just the Euclidean space $\mathbb{R}^n$ and that the base space of the fibre bundle is two dimensional, writing $(r_1, r_2; s_\alpha)$ for the coordinates. We will consider the class of nonholonomic systems where the Lagrangian is given by

$$L = \frac{1}{2}(I_1\dot{r}_1^2 + I_2\dot{r}_2^2 + \sum_\alpha I_\alpha \dot{s}_\alpha^2), \tag{13}$$

(with all I_α positive constants) and where the constraints take the following special form

$$\dot{s}_\alpha = -A_\alpha(r_1)\dot{r}_2. \tag{14}$$

Although this may seem to be a very thorough simplification, this interesting class of systems does include, for example, all the classical examples described above. We also remark that all of the above systems fall in the category of so-called Chaplygin systems (see [3]). The case of 2-dimensional distributions was also studied by Cartan, be it for other purposes (see e.g. [6] and the references therein).

In what follows, we will assume that none of the A_α are constant (in that case the constraints are, of course, holonomic). The nonholonomic equations of motion (1) are now

$$\ddot{r}_1 = 0, \quad \ddot{r}_2 = -N^2\big(\sum_\beta I_\beta A_\beta A'_\beta\big)\dot{r}_1\dot{r}_2, \quad \dot{s}_\alpha = -A_\alpha \dot{r}_2, \tag{15}$$

where N is shorthand for the function

$$N(r_1) = \frac{1}{\sqrt{I_2 + \sum_\alpha I_\alpha A_\alpha^2}}. \tag{16}$$

This function is directly related to the invariant measure of the system. Indeed, we have shown in [16] that for a two-degree of freedom system such as (15), we may compute the density N of the invariant measure (if it exists) by integrating two first-order partial differential equations derived from the condition that the volume form be preserved along the nonholonomic flow. In the present case, these two equations read:

$$\frac{1}{N}\frac{\partial N}{\partial r_1} + \frac{\sum_\beta I_\beta A_\beta A'_\beta}{I_2 + \sum_\alpha I_\alpha A_\alpha^2} = 0, \qquad \frac{1}{N}\frac{\partial N}{\partial r_2} = 0, \tag{17}$$

and obviously the expression for N in (16) is its solution up to an irrelevant multiplicative constant. In case of the free nonholonomic particle and the knife edge the invariant measure density is $N \sim 1/\sqrt{1+x^2}$ and $N \sim 1/\sqrt{(1+\tan^2(\phi))} = \cos(\phi)$, respectively. In case of the vertically rolling disk it is a constant. We shall see later that systems with a constant invariant measure (or equivalently, with constant $\sum_\alpha I_\alpha A_\alpha^2$) always play a somehow special role.

We are now in a position to generalize the associated second-order systems presented in section 2.1 to the more general class of nonholonomic systems above. In the set-up above, the first associated second-order system is, for the more general systems (15), the system

$$\ddot{r}_1 = 0, \quad \ddot{r}_2 = -N^2\big(\sum_\beta I_\beta A_\beta A'_\beta\big)\dot{r}_1\dot{r}_2, \quad \ddot{s}_\alpha = -(A'_\alpha \dot{r}_1\dot{r}_2 + A_\alpha \ddot{r}_2),$$

or equivalently, in normal form,

$$\begin{aligned} &\ddot{r}_1 = 0, \qquad\qquad \ddot{r}_2 = -N^2\big(\sum_\beta I_\beta A_\beta A'_\beta\big)\dot{r}_1\dot{r}_2, \\ &\ddot{s}_\alpha = -\Big(A'_\alpha - N^2 A_\alpha\big(\sum_\beta I_\beta A_\beta A'_\beta\big)\Big)\dot{r}_1\dot{r}_2. \end{aligned} \tag{18}$$

For convenience, we will often simply write

$$\ddot{r}_1 = 0, \quad \ddot{r}_2 = \Gamma_2(r_1)\dot{r}_1\dot{r}_2, \quad \ddot{s}_\alpha = \Gamma_\alpha(r_1)\dot{r}_1\dot{r}_2,$$

for these types of second-order systems.

The second associated second-order system we encountered for the vertically rolling disk also translates to the more general setting. We get

$$\begin{aligned} &\ddot{r}_1 = 0, \qquad\qquad \ddot{r}_2 = -N^2\big(\sum_\beta I_\beta A_\beta A'_\beta\big)\dot{r}_1\dot{r}_2, \\ &\ddot{s}_\alpha = \Big(A'_\alpha - N^2 A_\alpha\big(\sum_\beta I_\beta A_\beta A'_\beta\big)\Big)\dot{r}_1\left(\frac{\dot{s}_\alpha}{A_\alpha}\right), \end{aligned} \tag{19}$$

where in the right-hand side of the last equation, there is no sum over α. A convenient byproduct of this way of associating a second-order system to (15) is that now all equations decouple except for the coupling with the r_1-equation. To highlight this, we will write this system as

$$\ddot{r}_1 = 0, \quad \ddot{q}_a = \Xi_a(r_1)\dot{q}_a\dot{r}_1$$

(no sum over a) where, from now on, $(q_a) = (r_2, s_\alpha)$ and $(q_i) = (r_1, q_a)$.

We postpone the discussion about the third associated second-order system of our class until section 4.4.

4 Lagrangians for associated second-order systems

4.1 The inverse problem of Lagrangian mechanics

Let Q be a manifold with local coordinates (q^i) and assume we are given a system of second-order ordinary differential equations $\ddot{q}^i = f^i(q, \dot{q})$ on Q. The search for a regular Lagrangian is known in the literature as 'the inverse problem of the calculus of variations,' and has a long history (for a recent survey on this history, see e.g. [21] and the long list of references therein). In order for a regular Lagrangian $L(q, \dot{q})$ to exist we must be able to find functions $g_{ij}(q, \dot{q})$, so-called multipliers, such that

$$g_{ij}(\ddot{q}^j - f^j) = \frac{d}{dt}\left(\frac{\partial L}{\partial \dot{q}^i}\right) - \frac{\partial L}{\partial q^i}.$$

It can be shown [2, 12, 27] that the multipliers must satisfy

$$\begin{aligned}
&\det(g_{ij}) \neq 0, \qquad g_{ji} = g_{ij}, \qquad \frac{\partial g_{ij}}{\partial \dot{q}^k} = \frac{\partial g_{ik}}{\partial \dot{q}^j};\\
&\Gamma(g_{ij}) - \nabla^k_j g_{ik} - \nabla^k_i g_{kj} = 0,\\
&g_{ik}\Phi^k_j = g_{jk}\Phi^k_i;
\end{aligned}$$

where $\nabla^i_j = -\frac{1}{2}\partial_{\dot{q}^j} f^i$ and

$$\Phi^k_j = \Gamma\left(\partial_{\dot{q}^j} f^k\right) - 2\partial_{q^j} f^k - \frac{1}{2}\partial_{\dot{q}^j} f^l \partial_{\dot{q}^l} f^k.$$

The symbol Γ stands for the vector field $\dot{q}^i\partial_{q^i} + f^i\partial_{\dot{q}^i}$ on TQ that can naturally be associated to the system $\ddot{q}^i = f^i(q, \dot{q})$. Conversely, if one can find functions g_{ij} satisfying these conditions then the equations $\ddot{q}^i = f^i$ are derivable from a regular Lagrangian. Moreover, if a regular Lagrangian L can be found, then its Hessian $\dfrac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}$ is a multiplier.

The above conditions are generally referred to as the Helmholtz conditions. We will fix from the start $g_{ij} = g_{ji}$ for $j \leq i$, and we will simply write g_{ijk} for $\partial_{\dot{q}^k} g_{ij}$, and also assume the notation to be symmetric over all its indices.

The Helmholtz conditions are a mixed set of coupled algebraic and PDE conditions in (g_{ij}). We will refer to the penultimate condition as the '∇- condition,' and to the last one as the 'Φ-condition.' The algebraic Φ-conditions are of course the most interesting to start from. In fact, we can easily derive more algebraic conditions (see e.g. [11]). For example, by taking a Γ-derivative of the Φ-condition, and by replacing $\Gamma(g_{ij})$ everywhere by means of the ∇-condition, we arrive at a new algebraic condition of the form

$$g_{ik}(\nabla\Phi)^k_j = g_{jk}(\nabla\Phi)^k_i,$$

where $(\nabla\Phi)^i_j = \Gamma(\Phi^i_j) - \nabla^i_m\Phi^m_j - \nabla^m_j\Phi^i_m$. As in [11], we will call this new condition the $(\nabla\Phi)$-condition. It will, of course, only give new information as long as it is independent from the Φ-condition (this will not be the case, for example, if the commutator of matrices $[\Phi, \nabla\Phi]$ vanishes). One can repeat the above process on the $(\nabla\Phi)$-condition, and so on to obtain possibly independent $(\nabla\ldots\nabla\Phi)$-conditions.

A second route to additional algebraic conditions arises from the derivatives of the Φ-equation in $\dot q$-directions. One can sum up those derived relations in such a way that the terms in g_{ijk} disappear on account of the symmetry in all their indices. The new algebraic relation in g_{ij} is then of the form

$$g_{ij}R^j_{kl} + g_{lj}R^j_{ik} + g_{kj}R^j_{li} = 0,$$

where $R^j_{kl} = \partial_{\dot q^j}(\Phi^k_i) - \partial_{\dot q^i}(\Phi^k_j)$. For future use, we will call this the R-condition.

As before, this process can be continued to obtain more algebraic conditions. Also, any mixture of the above mentioned two processes leads to possibly new and independent algebraic conditions. Once we have used up all the information that we can obtain from this infinite series of algebraic conditions, we can start looking at the partial differential equations in the ∇-conditions.

We are now in a position to investigate whether a Lagrangian exists for the two choices of associated systems (18) and (19).

4.2 Lagrangians for the first associated second-order system

The first second-order system of interest is of the form

$$\ddot r_1 = 0, \quad \ddot r_2 = \Gamma_2(r_1)\dot r_1\dot r_2, \quad \ddot s_\alpha = \Gamma_\alpha(r_1)\dot r_1\dot r_2. \tag{20}$$

The only non-zero components of (Φ^i_j) are

$$\begin{aligned}
\Phi^2_1 &= (\frac{1}{2}\Gamma^2_2 - \Gamma'_2)\dot r_1\dot r_2, & \Phi^2_2 &= -(\frac{1}{2}\Gamma^2_2 - \Gamma'_2)\dot r_1^2,\\
\Phi^\alpha_1 &= (\frac{1}{2}\Gamma_\alpha\Gamma_2 - \Gamma'_\alpha)\dot r_1\dot r_2, & \Phi^\alpha_2 &= -(\frac{1}{2}\Gamma_\alpha\Gamma_2 - \Gamma'_\alpha)\dot r_1^2.
\end{aligned}$$

For $\nabla\Phi$ and $\nabla\nabla\Phi$ we get

$$\begin{aligned}
(\nabla\Phi)^2_1 &= (\Gamma_2\Gamma'_2 - \Gamma''_2)\dot r_1^2\dot r_2, & (\nabla\Phi)^2_2 &= -(\Gamma_2\Gamma'_2 - \Gamma''_2)\dot r_1^3,\\
(\nabla\Phi)^\alpha_1 &= (\Gamma_\alpha\Gamma_2 - \Gamma''_\alpha)\dot r_1^2\dot r_2, & (\nabla\Phi)^\alpha_2 &= -(\Gamma_\alpha\Gamma_2 - \Gamma''_\alpha)\dot r_1^3,
\end{aligned}$$

and

$$\begin{aligned}
(\nabla\nabla\Phi)^2_1 &= ((\Gamma'_2)^2 + \Gamma_2\Gamma''_2 - \Gamma'''_2)\dot r_1^3\dot r_2,\\
(\nabla\nabla\Phi)^2_2 &= -((\Gamma'_2)^2 + \Gamma_2\Gamma''_2 - \Gamma'''_2)\dot r_1^4\\
(\nabla\nabla\Phi)^\alpha_1 &= (\Gamma'_\alpha\Gamma'_2 + \frac{3}{2}\Gamma_\alpha\Gamma''_2 - \frac{1}{2}\Gamma''_\alpha\Gamma_2 - \Gamma'''_\alpha)\dot r_1^3\dot r_2,\\
(\nabla\nabla\Phi)^\alpha_2 &= -(\Gamma'_\alpha\Gamma'_2 + \frac{3}{2}\Gamma_\alpha\Gamma''_2 - \frac{1}{2}\Gamma''_\alpha\Gamma_2 - \Gamma'''_\alpha)\dot r_1^4,
\end{aligned}$$

and so on.

We can already draw some immediate consequences just by looking at the above explicit expressions. Let's make things a bit more accessible by considering the case where the dimension is 4. Then, the Φ-equations of the system (20) and their derivatives are all of the form

$$\begin{aligned}
&g_{12}\Psi_2^2 + g_{13}\Psi_2^3 + g_{14}\Psi_2^4 = g_{22}\Psi_1^2 + g_{23}\Psi_1^3 + g_{24}\Psi_1^4,\\
&g_{23}\Psi_1^2 + g_{33}\Psi_1^3 + g_{34}\Psi_1^4 = 0,\\
&g_{23}\Psi_2^2 + g_{33}\Psi_2^3 + g_{34}\Psi_2^4 = 0,\\
&g_{24}\Psi_1^2 + g_{34}\Psi_1^3 + g_{44}\Psi_1^4 = 0,\\
&g_{24}\Psi_2^2 + g_{34}\Psi_2^3 + g_{44}\Psi_2^4 = 0,
\end{aligned} \tag{21}$$

where, within the same equation, Ψ stands for either Φ, $\nabla\Phi$, $\nabla\nabla\Phi$, $\nabla\nabla\nabla\Phi$, ... We will refer to the equations of the first line in (21) as 'equations of the first type,' and to equations of the next four lines as 'equations of the second type.' The first 3 equations of the first type, namely those for Φ, $\nabla\Phi$ and $\nabla\nabla\Phi$ are explicitly:

$$\begin{aligned}
&g_{12}\Phi_2^2 + g_{13}\Phi_2^3 + g_{14}\Phi_2^4 = g_{22}\Phi_1^2 + g_{23}\Phi_1^3 + g_{24}\Phi_1^4,\\
&g_{12}(\nabla\Phi)_2^2 + g_{13}(\nabla\Phi)_2^3 + g_{14}(\nabla\Phi)_2^4 = g_{22}(\nabla\Phi)_1^2 + g_{23}(\nabla\Phi)_1^3 + g_{24}(\nabla\Phi)_1^4,\\
&g_{12}(\nabla\nabla\Phi)_2^2 + g_{13}(\nabla\nabla\Phi)_2^3 + g_{14}(\nabla\nabla\Phi)_2^4 = g_{22}(\nabla\nabla\Phi)_1^2 + g_{23}(\nabla\nabla\Phi)_1^3 + g_{24}(\nabla\nabla\Phi)_1^4.
\end{aligned} \tag{22}$$

For the systems at hand, the particular expression of Φ and its derivatives are such that

$$\begin{aligned}
&\Phi_2^2(\nabla\Phi)_1^2 - \Phi_1^2(\nabla\Phi)_2^2 = 0,\\
&(\nabla\Phi)_2^2(\nabla\nabla\Phi)_1^2 - (\nabla\Phi)_1^2(\nabla\nabla\Phi)_2^2 = 0,
\end{aligned}$$

and so on. By taking the appropriate linear combination of the first and the second, and of the second and the third equation in (22), we can therefore obtain two equations in which the unknowns g_{12} and g_{22} are eliminated. Moreover, under certain regularity conditions, these two equations can be solved for g_{13} and g_{14} in terms of g_{23} and g_{24} (we will deal with exceptions later on). So, if we can show that g_{23} and g_{24} both vanish, then so will also g_{13} and g_{14}. Then, in that case $g_{12}\Psi_2^2 = g_{22}\Psi_1^2$, but no further relation between g_{12} and g_{22} can be derived from this type of algebraic conditions.

The infinite series of equations given by those of the second type in (21) are all equations in the 5 unknowns g_{23}, g_{33}, g_{34}, g_{24} and g_{44}. Not all of these equations are linearly independent, however. In fact, given that the system (20) exhibits the property

$$\Psi_1^a\Psi_2^b - \Psi_1^b\Psi_2^a = 0,$$

(where Ψ is one of $\Phi, \nabla\Phi, \nabla\nabla\Phi, ...$), one can easily deduce that the last four lines of equations in (21) actually reduce to only two kinds of equations. If we assume that we can find among this infinite set 5 linearly independent equations, there will only be the zero solution

$$g_{23} = g_{33} = g_{34} = g_{24} = g_{44} = 0,$$

and from the previous paragraph we know that then also $g_{14} = g_{13} = 0$. To conclude, under the above mentioned assumptions, the matrix of multipliers

$$(g_{ij}) = \begin{pmatrix} g_{11} & g_{12} & 0 & 0\\ g_{12} & g_{22} & 0 & 0\\ 0 & 0 & 0 & 0\\ 0 & 0 & 0 & 0 \end{pmatrix}$$

is singular and we conclude that there is no regular Lagrangian for the system. The above reasoning can, of course, be generalized to lower and higher dimensions.

We will refer to the above as 'the general case'. The assumptions made above are, however, not always satisfied, and they need to be checked for every particular example. Let us consider first the example of the (three-dimensional) nonholonomic particle, where $\Gamma_2 = -x/(1+x^2)$ and $\Gamma_3 = -1/(1+x^2)$. The equations for $\Psi = \Phi, \nabla\Phi$ of the second type give the following two linear independent equations

$$(\dot{x}^2 - 2)g_{23} + 3xg_{33} = 0, \quad (x^3 - 5x)g_{23} + (5x^2 - 1)g_{33} = 0.$$

We can easily conclude that $g_{23} = g_{33} = 0$. With that, the first two equations of the first type are

$$\begin{aligned}&(x^2-2)\dot{x}g_{12} + 3x\dot{x}g_{13} + (x^2-2)\dot{y}g_{22} = 0,\\&(x^3-5x)\dot{x}g_{12} + (5x^2-1)\dot{x}g_{13} + (x^3-5x)\dot{y}g_{22}.\end{aligned}$$

From this $g_{13} = 0$ and $\dot{x}g_{12} = -\dot{y}g_{22}$, and there is therefore no regular Lagrangian.

With a similar reasoning (but with different coefficients) we reach the same conclusion for the example of the knife edge on a plane.

The vertically rolling disk is a special case, however, and so is any system (15) with the property that $\sum_\alpha I_\alpha A_\alpha^2$ is a constant. This last relation is in fact equivalent with the geometric assumption that the density of the invariant measure N is constant. In that case, we get $\Gamma_2 = 0$. Not only does Γ_2 vanish, but so do all Ψ_1^2 and Ψ_2^2 for $\Psi = \Phi, \nabla\Phi, \ldots$. We also have $\Gamma_3 = -R\sin(\varphi)$ and $\Gamma_4 = R\cos(\varphi)$. Moreover, looking again first at expressions (22), one can easily show that for the vertically rolling disk these three equations, and in fact any of the equations that follow in that series, are all linearly depending on the following two equations

$$\begin{aligned}&\cos(\varphi)\dot{\varphi}g_{13} + \sin(\varphi)\dot{\varphi}g_{14} + \cos(\varphi)\dot{\theta}g_{23} + \sin(\varphi)\dot{\theta}g_{24} = 0,\\&\sin(\varphi)\dot{\varphi}g_{13} - \cos(\varphi)\dot{\varphi}g_{14} + \sin(\varphi)\dot{\theta}g_{23} - \cos(\varphi)\dot{\theta}g_{24} = 0.\end{aligned}$$

Although these equations are already in a form where g_{12} and g_{22} do not show up, it is quite inconvenient that there is no way to relate these two unknowns to any of the other unknowns. However, as in the general case, we can deduce from this an expression for g_{13} and g_{14} as a function of g_{23} and g_{24}. We get

$$g_{13} = -\frac{\dot{\theta}}{\dot{\varphi}}g_{23}, \qquad g_{14} = -\frac{\dot{\theta}}{\dot{\varphi}}g_{24}. \tag{23}$$

The infinite series of equations of the second type (i.e. the last four lines in (21)) are all linearly dependent to either one of the following four equations

$$\begin{aligned}&\cos(\varphi)g_{33} + \sin(\varphi)g_{34} = 0, \quad \cos(\varphi)g_{34} + \sin(\varphi)g_{44} = 0\\&\sin(\varphi)g_{33} - \cos(\varphi)g_{34} = 0, \quad \sin(\varphi)g_{34} - \cos(\varphi)g_{44} = 0,\end{aligned}$$

from which $g_{33} = g_{34} = g_{44} = 0$ follows immediately. In comparison to the general case, however, we can no longer conclude from the above that also g_{23} and g_{24} vanish, and therefore, we can also not conclude from (23) that g_{13} and g_{14} vanish. This concludes, in fact, the information we can extract from the Φ-condition, and the algebraic conditions that follow from taking its derivatives w.r.t. ∇. Also, any attempt to create new algebraic conditions by means of the tensor R is fruitless, since an easy calculation shows that, when the above conclusions are taken already into account, all equations that can be derived from R are automatically satisfied. However, we have enough information to conclude that there does not exist a regular Lagrangian for the vertically rolling disk and its first associated second-order system. Indeed, the determinant of the multiplier matrix

$$(g_{ij}) = \begin{pmatrix} g_{11} & g_{12} & \lambda g_{23} & \lambda g_{24} \\ g_{12} & g_{22} & g_{23} & g_{24} \\ \lambda g_{23} & g_{23} & 0 & 0 \\ \lambda g_{24} & g_{24} & 0 & 0 \end{pmatrix},$$

(with $\lambda = -\dot{\theta}/\dot{\varphi}$) clearly vanishes and this is a violation of one of the first Helmholtz conditions.

Thus, to summarize the above results, for the nonholonomic free particle (2), the knife edge on the plane (4) and the vertically rolling disk (5), we conclude that there does not exist a regular Lagrangian for their first associated second-order system (18).

4.3 Lagrangians for the second associated second-order system

In this section, we will investigate the inverse problem for the second associated system,

$$\ddot{r}_1 = 0, \qquad \ddot{q}_a = \Xi_a(r_1)\dot{q}_a\dot{r}_1. \tag{24}$$

In the q_a-equations, there is no sum over a, which is an index that runs from 2 to the dimension of the configuration space, and with respect to the formulation of the inverse problem in section 3, we have $f_1 = 0$ and $f_a = \Xi_a\dot{q}_a\dot{r}_1$. Moreover, one can easily compute that the only non-vanishing components of Φ are now

$$\Phi^a_1 = -\frac{1}{2}\dot{r}_1\dot{q}_a(2\Xi'_a - \Xi_a^2), \quad \Phi^a_a = \frac{1}{2}\dot{r}_1^2(2\Xi'_a - \Xi_a^2).$$

The Φ-conditions turn out to be quite simple: if $\Phi^a_a \neq 0$, then

$$\dot{q}_a g_{aa} = -\dot{r}_1 g_{1a}, \tag{25}$$

and if $\Phi^a_a \neq \Phi^b_b$ for $a \neq b$, then

$$g_{ab} = 0. \tag{26}$$

These restrictions on Φ lead to the assumptions that first $\Xi_a \neq 0$ and $\Xi_a \neq 2/(C - r_1)$, where C is any constant, second that $\Xi_a \neq \Xi_b$ and, formally, $\Xi_a - \Xi_b \neq E_b/(C - \int E_b dr_1)$, where $E_b(r_1) = \exp(\int 2\Xi_b dr_1)$. Suppose for now that we are dealing with nonholonomic systems (19) where this is the case. Then one can easily show that all the other $\nabla \ldots \nabla\Phi$-conditions do not contribute any new information, as well as that the R-condition is automatically satisfied. Thus we should therefore turn our attention to the ∇-condition, which is a PDE. To simplify the subsequent analysis though, we note that although the multipliers g_{ij} can in general be functions of all variables $(r_1, q_a, \dot{r}_1, \dot{q}_a)$, in view of the symmetry of the system we shall assume them to be, without loss of generality, functions of $(r_1, \dot{r}_1, \dot{q}_a)$ only.

Now, by differentiating the algebraic conditions by r_1, $\dot{r}_1$ and $\dot{q}_a$, we get the additional conditions

$$\begin{aligned} &\dot{q}_a g'_{aa} = -\dot{r}_1 g'_{1a} \\ &g_{aa} + \dot{q}_a g_{aaa} = -\dot{r}_1 g_{1aa}, \quad \dot{q}_a g_{1aa} = -g_{1a} - \dot{r}_1 g_{11a} \\ &g_{aab} = 0 = g_{1ab}, \quad \text{if } a \neq b. \end{aligned}$$

Finally, the ∇-Helmholtz conditions are, with the above already incorporated,

$$g'_{11} + \sum_b \Xi_b (g_{11b}\dot{q}_b - g_{bb}\frac{\dot{q}_b^2}{\dot{r}_1^2}) = 0,$$
$$g'_{aa} + \Xi_a (g_{aaa}\dot{q}_a + g_{aa}) = 0.$$

In what follows we will implicitly assume everywhere that $\dot{r}_1 \neq 0$. As a consequence, the multipliers (g_{ij}) (and the Lagrangians we may derive from it) will only be defined for $\dot{r}_1 \neq 0$

It is quite impossible to find the most general solution for (g_{ij}) though. We will show that there is an interesting class of solutions if we make the anszatz that $g_{bbb} = 0$ for all b. With that and with the above $g_{aab} = 0$ in mind, we conclude that all such g_{bb} will depend only on possibly r_1 and $\dot{r}_1$. Moreover, from the last ∇-conditions we can determine their dependency on the variable r_1. Since now

$$g'_{bb} + g_{bb}\Xi_b = 0,$$

it follows that $g_{bb}(r_1, \dot{r}_1) = F_b(\dot{r}_1)\exp(-\xi_b(r_1))$, where ξ_b is such that $\xi'_b = \Xi_b$ and where $F_b(\dot{r}_1)$ is still to be determined from the remaining conditions. From one of the above conditions we get $g_{1bb} = -g_{bb}/\dot{r}_1$ (since $g_{bbb} = 0$), so

$$\frac{dF_b}{d\dot{r}_1} = -\frac{F_b}{\dot{r}_1},$$

from which $F_b = C_b/\dot{r}_1$, with C_b a constant, and thus $g_{bb} = C_b \exp(-\xi_b)/\dot{r}_1$. Therefore, from the algebraic conditions, $g_{1b} = -(g_{bb}/\dot{r}_1)\dot{q}_b = -C_b \exp(-\xi_b)\dot{q}_b/\dot{r}_1^2$, and thus $g_{11b} = 2C_b\dot{q}_b \exp(-\xi_b)/\dot{r}_1^3$. With this, the first ∇-condition becomes

$$g'_{11} + \sum_b C_b \exp(-\xi_b)\xi'_b \frac{\dot{q}_b^2}{\dot{r}_1^3} = 0,$$

and thus

$$g_{11} = \sum_b C_b \exp(-\xi_b)\frac{\dot{q}_b^2}{\dot{r}_1^3} + C(\dot{r}_1, \dot{q}_b).$$

Given that $g_{11b} = 2C_b\dot{q}_b \exp(-\xi_b)/\dot{r}_1^3$, we can now determine the $\dot{q}_b$-dependence of C. We simply get

$$g_{11} = \sum_b C_b \exp(-\xi_b)\frac{\dot{q}_b^2}{\dot{r}_1^3} + F_1(\dot{r}_1).$$

Notice that g_{111} does not show up explicitly in the conditions or in the derived conditions. Therefore, there will always be some freedom in the g_{11}-part of the Hessian, represented here by the undetermined function $F_1(\dot{r}_1)$.

Up to a total time derivative, the most general Lagrangian whose Hessian $g_{ij} = \dfrac{\partial^2 L}{\partial \dot{q}^i \partial \dot{q}^j}$ is the above multiplier, is:

$$L = \rho(\dot{r}_1) + \frac{1}{2}\sum_b C_b \exp(-\xi_b)\frac{\dot{q}_b^2}{\dot{r}_1}, \tag{27}$$

where $d^2\rho/d\dot{r}_1^2 = F_1$. One can easily check that the Lagrangian is regular, as long as $d^2\rho/d\dot{r}_1^2$ is not zero, and as long as none of the C_b are zero. Remark, finally, that the Lagrangian is only defined on the whole tangent space if $C_b = 0$ (and ρ is at least C^2 everywhere). We can therefore only conclude that there is a regular Lagrangian (with the ansatz $g_{bbb} = 0$) on that part of the tangent manifold where $\dot r_1 \neq 0$. As a consequence, the solution set of the Euler-Lagrange equations of the Lagrangian (27) will not include those solutions of the second-order system (20) where $\dot r_1 = 0$. In case of the vertically rolling disk, for example, these solutions are exactly the special ones given by (7), and that is the reason why we will exclude them from our formalism.

Recall that at the beginning of this section, we have made the assumptions that $\Phi^a_a \neq 0$ and $\Phi^a_a \neq \Phi^b_b$. Suppose now that one of these assumptions is not valid, say $\Xi_2 = 0$ and therefore $\Phi^2_2 = 0$. Then, among the algebraic Helmholtz conditions there will no longer be a relation in (25) that links g_{22} to g_{12}. In fact, since the g_{ij} now need to satisfy only a smaller number of algebraic conditions, the set of possible Lagrangians may be larger. We can, of course, still take the relation

$$\dot q_2 g_{22} = -\dot r_1 g_{12} \tag{28}$$

as an extra ansatz (rather than as a condition) and see whether there exists Lagrangians with that property. By following the same reasoning as before, we easily conclude that the function (27) is also a Lagrangian for systems with $\Phi^2_2 = 0$. In fact, it will be a Lagrangian if any of the assumptions is not valid.

Apart from (28), we are, of course, free to take any other ansatz on g_{12} and g_{22}. If we simply set

$$g_{12} = 0,$$

it can easily be verified that also

$$L = \rho(\dot r_1) + \sigma(\dot r_2) + \frac{1}{2}\left(\sum_\alpha a_\alpha \exp(-\xi_\alpha)\frac{\dot s_\alpha^2}{\dot r_1}\right) \tag{29}$$

is a Lagrangian for a system (24) with $\Xi_2 = 0$ (where, as usual, $(q_a) = (r_2, s_\alpha)$). It is regular as long as both $d^2\rho/d\dot r_1^2$ and $d^2\sigma/d\dot r_2^2$ do not vanish.

Proposition 1. *The function*

$$L = \rho(\dot r_1) + \frac{1}{2N}\left(C_2\frac{\dot r_2^2}{\dot r_1} + \sum_\beta C_\beta \frac{\dot s_\beta^2}{A_\beta \dot r_1}\right), \tag{30}$$

with $d^2\rho/d\dot r_1^2 \neq 0$ and all $C_\alpha \neq 0$ is in any case a regular Lagrangian for the second associated systems (19). If the invariant measure density N is a constant, then also

$$L = \rho(\dot r_1) + \sigma(\dot r_2) + \frac{1}{2N}\sum_\beta a_\beta \frac{\dot s_\beta^2}{A_\beta \dot r_1}, \tag{31}$$

where $d^2\rho/d\dot r_1^2 \neq 0$, $d^2\sigma/d\dot r_1^2 \neq 0$ and all $C_\alpha \neq 0$ is a regular Lagrangian for the second associated systems (19).

Proof. For the second associated systems, the second-order equations (24) are of the form (19). One easily verifies that in that case

$$\xi_2 = \ln N \quad \text{and} \quad \xi_\alpha = \ln(N A_\alpha) \tag{32}$$

are such that $\xi'_a = \Xi_a$. The first Lagrangian in the theorem is then equal to the one in (27). For a system with constant invariant measure N, we get that $\Xi_2 = 0$. Therefore, also the function (29) is a valid Lagrangian. □

Let us end this section with a list of the Lagrangians for the nonholonomic free particle, the knife edge on a horizontal plane and the vertically rolling disk. The respective Lagrangians (30) for the first two examples are:

$$L = \rho(\dot{x}) + \frac{1}{2}\sqrt{1+x^2}\left(C_2\frac{\dot{y}^2}{\dot{x}} + C_3\frac{\dot{z}^2}{x\dot{x}}\right), \tag{33}$$

and

$$\begin{aligned} L &= \rho(\dot{\phi}) + \frac{1}{2}\sqrt{m(1+\tan(\phi)^2)}\left(C_2\frac{\dot{x}^2}{\dot{\phi}} + C_3\frac{\dot{y}^2}{\tan(\phi)\dot{\phi}}\right), \\ &= \rho(\dot{\phi}) + \frac{1}{2}C_2\sqrt{m}\frac{\dot{x}^2}{\cos(\phi)\dot{\phi}} + \frac{1}{2}C_3\sqrt{m}\frac{\dot{y}^2}{\sin(\phi)\dot{\phi}}. \end{aligned} \tag{34}$$

The vertically rolling disk in one of those systems with constant invariant measure. The first Lagrangian (30) is:

$$L = \rho(\dot{\varphi}) + \frac{\sqrt{I+mR^2}}{2}\left(C_2\frac{\dot{\theta}^2}{\dot{\varphi}} + C_3\frac{\dot{x}^2}{\cos(\varphi)\dot{\varphi}} + C_4\frac{\dot{y}^2}{\sin(\varphi)\dot{\varphi}}\right) \tag{35}$$

and the second Lagrangian (31) is:

$$L = \rho(\dot{\varphi}) + \sigma(\dot{\theta}) - \frac{\sqrt{I+mR^2}}{2}\left(a_3\frac{\dot{x}^2}{\cos(\varphi)\dot{\varphi}} + a_4\frac{\dot{y}^2}{\sin(\varphi)\dot{\varphi}}\right). \tag{36}$$

4.4 Lagrangians for the third associated second-order system

In section 2.1 we have described a third associated second-order system (11) for the example of the vertically rolling disk. That system comes actually from a comparison of the variational nonholonomic and the Lagrange-d'Alembert nonholonomic equations of motion we conducted in [16]. There we investigated the conditions under which the variational nonholonomic Lagrangian L_V would reproduce the nonholonomic equations of motion when restricted to the nonholonomic constraint manifold. Thus, instead of associating second-order systems to nonholonomic equations and applying the techniques of the inverse problem to derive the Lagrangian (and the Hamiltonian), in [16] we started from a specific Lagrangian (the variational nonholonomic Lagrangian L_V) and investigated the conditions under which its variational equations match the nonholonomic equations. Other relevant work on this matter can be found in e.g. [8].

In case of our class of nonholonomic systems with Lagrangian (13) and constraints (14) the variational nonholonomic Lagrangian is simply

$$\begin{aligned} L_V &= L - \sum_\alpha \frac{\partial L}{\partial \dot{s}_\alpha}(\dot{s}_\alpha + A_\alpha \dot{r}_2) \\ &= \frac{1}{2}(I_1\dot{r}_1^2 + I_1\dot{r}_1^2 - \sum_\alpha I_\alpha \dot{s}_\alpha^2) - \sum_\alpha A_\alpha I_\alpha \dot{s}_\alpha \dot{r}_2. \end{aligned}$$

A short calculation shows that its Euler-Lagrange equations in normal form are given by

$$\begin{aligned} &\ddot{r}_1 = -\big(\sum_\beta I_\beta A'_\beta \dot{s}_\beta\big)\dot{r}_2, \qquad \ddot{r}_2 = -N^2\big(\sum_\beta I_\beta A_\beta A'_\beta\big)\dot{r}_1\dot{r}_2 + \big(\sum_\beta I_\beta A'_\beta \dot{s}_\beta\big)\dot{r}_1, \\ &\ddot{s}_\alpha = -\Big(A'_\alpha - N^2 A_\alpha\big(\sum_\beta I_\beta A_\beta A'_\beta\big)\Big)\dot{r}_1\dot{r}_2 - A_\alpha\big(\sum_\beta I_\beta A'_\beta \dot{s}_\beta\big)\dot{r}_1. \end{aligned} \tag{37}$$

In general, these systems are not associated to our class of nonholonomic systems. That is, the restriction of their solutions to the constraint manifold $\dot{s}_\alpha = -A_\alpha \dot{r}_2$ are not necessarily solutions of the nonholonomic equations (15). However, in case that the invariant measure density N is a constant, we have that $\sum_\beta I_\beta A_\beta A'_\beta = 0$. As a consequence, all the terms in the equations (37) that contain $\sum_\beta I_\beta A'_\beta \dot{s}_\beta$ vanish when we restrict those equations to the constraint manifold and the equations in $\ddot{s}_\alpha$ integrate to the equations of constraint (14). The restriction of the equations (37) is therefore equivalent with the nonholonomic equations (15). We conclude the following.

Proposition 2. *If N is constant, the equations (37) form an associated second-order system and, by construction, they are equivalent to the Euler-Lagrange equations of the variational nonholonomic Lagrangian L_V.*

We refer to [16] for more details and some more general statements on this way of finding a Lagrangian for a nonholonomic system and we end the discussion on the third associated systems here.

5 Hamiltonian formulation and the constraints in phase space

In the situations where we have found a regular Lagrangian, the Legendre transformation leads to an associated Hamiltonian system. Since the base solutions of the Euler-Lagrange equations of a regular Lagrangian are also base solutions of Hamilton's equations of the corresponding Hamiltonian, the Legendre transformation FL will map those solutions of the Euler-Lagrange equations that lie in the constraint distribution $\mathcal{D}$ to solutions of the Hamilton equations that belong to the constraint manifold $\mathcal{C} = FL(\mathcal{D})$ in phase space. Recall however that the Lagrangians for the second associated second-order systems (and their Legendre transformation) were not defined on $\dot{r}_1 = 0$, and so will also the corresponding Hamiltonians.

Let us put for convenience $\rho(\dot{r}_1) = \frac{1}{2} I_1 \dot{r}_1^2$ and $\sigma(\dot{r}_2) = \frac{1}{2} I_2 \dot{r}_2^2$ in the Lagrangians of the previous section.

Proposition 3. *Given the second associated second-order system (19), the regular Lagrangian (30) (away from $\dot{r}_1 = 0$) and constraints (14) on TQ are mapped by the Legendre transform to the Hamiltonian and constraints in T^*Q given by:*

$$H = \frac{1}{2I_1}\left(p_1 + \frac{1}{2}N\left(\frac{p_2^2}{C_2} + \sum_\beta A_\beta \frac{p_\beta^2}{C_\beta}\right)\right)^2, \qquad C_2 p_\alpha = -C_\alpha p_2. \tag{38}$$

In case N is constant, the second Lagrangian (31) and constraints (14) are transformed into

$$H = \frac{1}{2I_2}p_2^2 + \frac{1}{2I_1}\left(p_1 + \frac{1}{2}N\left(\sum_\beta \frac{A_\beta}{a_\beta}p_\beta^2\right)\right)^2, \quad I_2 N \dot{r}_1 p_\alpha + a_\alpha p_2 = 0, \tag{39}$$

where $\dot{r}_1(r_1, p_1, p_\alpha) = (p_1 + \frac{1}{2}N\sum_\alpha A_\alpha p_\alpha^2/a_\alpha)/I_1$.

Proof. The Legendre transformation gives for the Lagrangian (27)

$$p_1 = I_1\dot{r}_1 - \frac{1}{2}\sum_b C_b \exp(-\xi_b)\frac{\dot{q}_b^2}{\dot{r}_1^2}, \qquad p_b = C_b \exp(-\xi_b)\frac{\dot{q}_b}{\dot{r}_1}, \tag{40}$$

from which one can easily verify that the corresponding Hamiltonian is

$$H = \frac{1}{2I_1}\left(p_1 + \frac{1}{2}\sum_b \exp(\xi_b)\frac{p_b^2}{C_b}\right)^2. \tag{41}$$

In the case of the second associated second-order systems in the form (19), the ξ_a take the form (32), and we obtain the Hamiltonian in expression (38). From (40) we can then compute the constraint manifold $\mathcal{C}$ in phase space. Since now

$$p_2 = C_2\frac{\dot r_2}{N\dot r_1} \quad \text{and} \quad p_\alpha = C_\alpha\frac{\dot q_\alpha}{N\dot r_1},$$

the constraints (14) can be rewritten as

$$\dot r_1\left(\frac{p_\alpha}{C_\alpha} + \frac{p_2}{C_2}\right) = 0,$$

where $\dot r_1 = \frac{1}{I_1}(p_1 + \frac{1}{2}N(p_2\dot r_2^2/C_2 + \sum_\beta A_\beta p_\beta^2/C_\beta))$. Assuming as always that $\dot r_1 \neq 0$, we get that the constraint manifold in phase space is given by $C_2 p_\alpha = -C_\alpha p_2$ for all α.

An analogous calculation with the Lagrangian (31) gives the Hamiltonian and the constraints in (39), in the case where N is constant. $\square$

We can recover the Hamiltonians of [17] from Proposition 2. As perhaps the simplest example, note that with $(r_1, r_2, s_\alpha) = (x, y, z)$, by taking C_2 and C_3 both to be 1, and $A(r_1) = x$, we recover the Hamiltonian and the constraint that appears in [17] for the nonholonomic free particle.

Consider now the knife edge on the plane. Taking $C_2 = C_3 = 1/\sqrt{m}$ and $A(\phi) = -\tan(\phi)$ gives:

$$H = \frac{1}{2J}\left(p_\phi + \frac{1}{2}(\cos(\phi)p_x^2 - \sin(\phi)p_y^2)\right)^2, \tag{42}$$

while the constraint manifold becomes

$$p_x + p_y = 0. \tag{43}$$

For the rolling disk we get for the first Hamiltonian (38)

$$H = \frac{1}{2J}\left(p_\varphi + \frac{1}{2\sqrt{I+mR^2}}\left(\frac{p_\theta^2}{C_2} - \frac{\cos(\varphi)p_x^2}{C_3} - \frac{\sin(\varphi)p_y^2}{C_4}\right)\right)^2,$$

and $C_2 p_x = -C_3 p_\theta$ and $C_2 p_y = -C_4 p_\theta$ for the constraints. These are not the Hamiltonian and the constraints that appear in [17] though. It turns out that the Hamiltonian and the constraints in [17] are in fact those that are associated to the second Hamiltonian (39). It is, with, for example, $a_3 = a_4 = -J/\sqrt{I+mR^2}$ of the form

$$H = \frac{1}{2I}p_\theta^2 + \frac{1}{2}\left(p_\varphi + \frac{1}{2}p_x^2\cos(\varphi) + \frac{1}{2}p_y^2\sin(\varphi)\right)^2$$

and the constraints are

$$\dot\varphi p_x = p_\theta, \qquad \dot\varphi p_y = p_\theta$$

where $\dot\varphi = p_\varphi + \frac{1}{2}\cos(\varphi)p_x^2 + \frac{1}{2}\sin(\varphi)p_y^2$ or, equivalently,

$$p_x - p_y = 0, \qquad \dot\varphi p_x - p_\theta = 0,$$

as the constraints appears in [17].

6 Pontryagin's Maximum Principle

Consider the optimal control problem of finding the controls u that minimize a given cost function $G(x,u)$ under the constraint of a first order controlled system $\dot{x}=f(x,u)$. One of the hallmarks of continuous optimal control problems is that, under certain regularity assumptions, the optimal Hamiltonian can be found by applying the Pontryagin maximum principle. Moreover, in most cases of physical interest, the problem can be rephrased so as to be solved by using Lagrange multipliers p. Form the Hamiltonian $H^P(x,p,u)=\langle p, f(x,u)\rangle - p_0 G(x,u)$ and calculate, if possible, the function $u^*(x,p)$ that satisfies the optimality conditions

$$\frac{\partial H^P}{\partial u}(x,p,u^*(x,p)) \equiv 0.$$

Then, an extremal $x(t)$ of the optimal control problem is also a base solution of Hamilton's equations for the optimal Hamiltonian given by $H^*(x,p)=H^P(x,p,u^*(x,p))$. The optimal controls $u^*(t)$ then follow from substituting the solutions $(x(t),p(t))$ of Hamilton's equations for H^* into $u^*(x,q)$.

Such a usage of the multiplier approach can also be applied with succes to the mechanics of physical systems with holonomic constraints. However, in the case of nonholonomically constrained systems the Lagrange multiplier approach, also called the *vakonomic* approach by Arnold [1], generally leads to dynamics that do not reproduce the physical equations of motion (see [8, 22] and references therein). Thus, the rich interplay between Pontryagin's Maximum Principle, the vakonomic approach, and the physical equations of motion of a constrained system breaks down when the constraints are nonholonomic. However as we showed in a previous paper [16], for certain systems and initial data the vakonomic approach and Lagrange-D'Alembert principle yield equivalent equations of motion.

We will show here for the second associated systems

$$\ddot{r}_1 = 0, \qquad \ddot{q}_a = \Xi_a(r_1)\dot{q}_a\dot{r}_1,$$

that we can also find the Hamiltonians of the previous section via a rather ad hoc application of Pontryagin's Maximum Principle. Hereto, let us put $\Xi_a=\xi_a'$ as before and observe that the above second-order system can easily be solved for $(\dot{r}_1(t),\dot{q}_a(t))$. Indeed, obviously $\dot{r}_1$ is constant along solutions, say u_1. We will suppose as before that $u_1\neq 0$. From the q_a-equations it also follows that $\dot{q}_a/\exp(\xi_a)$ is constant, and we will denote this constant by u_a. To conclude,

$$\dot{r}_1(t)=u_1, \quad \dot{q}_a(t)=u_a\exp(\xi_a(r_1(t))).$$

Keeping that in mind, we can consider the following *associated controlled first-order system*

$$\dot{r}_1=u_1, \quad \dot{q}_a=u_a\exp(\xi_a(r_1)) \tag{44}$$

(no sum over a), where (u_1,u_a) are now interpreted as controls.

The next proposition relates the Hamiltonians of Proposition 2 to the optimal Hamiltonians for the optimal control problem of certain cost functions, subject to the constraints given by the controlled system (44).

Proposition 4. *The optimal Hamiltonian H^* of the optimal control problem of minimizing the cost function*

$$G_1(r_1,q_a,u_1,u_a)=\frac{1}{2}\left(I_1u_1^2+\sum_a C_a\exp(\xi_a(r_1))\frac{u_a^2}{u_1}\right)$$

subject to the dynamics (44) is given by:

$$H^*(q,p) = \frac{1}{2I_1}\left(p_{r_1} + \frac{1}{2}\sum_b \exp(\xi_b)\frac{p_b^2}{C_b}\right)^2. \tag{45}$$

If Ξ_2 is zero, the optimal Hamiltonian for the optimal control problem of minimizing the cost function

$$G_2(r_1, q_a, u_1, u_a) = \frac{1}{2}\left(I_1 u_1^2 + I_2 u_2^2 + \sum_\alpha a_\alpha \exp(\xi_\alpha(r_1))\frac{u_\alpha^2}{u_1}\right),$$

subject to the dynamics (44) is given by:

$$H^*(q,p) = \frac{1}{2I_2}p_2^2 + \frac{1}{2I_1}\left(p_1 + \frac{1}{2}\sum_\beta \exp(\xi_\beta)\frac{p_\beta^2}{a_\beta}\right)^2. \tag{46}$$

In case the controlled system is associated to a nonholonomic system (that is, in case the ξ_a take the form (32)), the above Hamiltonians are respectively the Hamiltonians (38) and (39) of Proposition 2.

Proof. The Hamiltonian H^P is

$$H^P(r_1, q_a, p_1, p_a, u_1, u_a) = p_1 u_1 + \sum_a p_a u_a \exp(\xi_a) - G_1. \tag{47}$$

The optimality conditions $\partial H^P/\partial u_1 = 0$, $\partial H^P/\partial u_a = 0$, together with the assumption that $u_1 \neq 0$, yield the following optimal controls as functions of (q,p):

$$\begin{aligned} I_1 u_1^* &= p_1 + \frac{1}{2}\sum_a \exp(\xi_a)\frac{p_a^2}{C_a}, \\ \frac{u_a^*}{u_1^*} &= \frac{p_a}{C_a}. \end{aligned}$$

For the Hamiltonian $H^*(q,p) = H^P(q,p,u^*(q,p))$, we get

$$\begin{aligned} H^*(q,p) &= \left(p_1 - \frac{1}{2}I_1 u_1^*\right)u_1^* + \sum_a \exp(\xi_a)u_a^*\left(p_a - \frac{1}{2}C_a\frac{u_a^*}{u_1^*}\right) \\ &= \frac{1}{I_x}\left[\left(\frac{1}{2}p_1 - \frac{1}{4}\sum_a \exp(\xi_a)\frac{p_a^2}{C_a}\right)\left(p_1 + \frac{1}{2}\sum_b \exp(\xi_b)\frac{p_b^2}{C_b}\right)\right. \\ &\qquad\qquad \left. + \frac{1}{2}\sum_a \exp(\xi_a)\frac{p_a^2}{C_a}\left(p_1 + \frac{1}{2}\sum_b \exp(\xi_b)\frac{p_b^2}{C_b}\right)\right] \\ &= \frac{1}{2I_1}\left(p_1 + \frac{1}{2}\sum_b \exp(\xi_b)\frac{p_b^2}{C_b}\right)^2, \end{aligned}$$

which is exactly the Hamiltonian (41).

For the second cost function, with $\Xi_2 = 0$, we get for Pontryagin's Hamiltonian

$$H^P = p_{r_1}u_{r_1} + p_{r_2}u_{r_2} + \sum_\alpha p_\alpha u_\alpha \exp(\xi_\alpha) - G_2.$$

The optimal controls as functions of (q,p) are now

$$
\begin{aligned}
I_1 u^*_{r_1} &= p_{r_1} + \frac{1}{2}\sum_\alpha \exp(\xi_\alpha)\frac{p_\alpha^2}{a_\alpha}, \\
I_2 u^*_{r_2} &= p_{r_2}, \\
\frac{u^*_\alpha}{u^*_{r_1}} &= \frac{p_\alpha}{C_\alpha}.
\end{aligned}
$$

With this the Hamiltonian becomes

$$
H^*(q,p) = \frac{1}{2I_2}p_{r_2}^2 + \frac{1}{2I_1}\left(p_{r_1} + \frac{1}{2}\sum_\beta \exp(\xi_\beta)\frac{p_\beta^2}{a_\beta}\right)^2,
$$

which is exactly (39) after the substitution (32). □

7 Related Research Directions and Conclusions

In essence, the method we have introduced in the previous sections resulted in an unconstrained, variational system which when restricted to an appropriate submanifold reproduces the dynamics of the underlying nonholonomic system. Although we have restricted our attention to a certain explicit subclass of nonholonomic systems, many of the more geometric aspects of the introduced method seem to open the door to generalizing the results to larger classes of systems. For example, a lot of what has been discussed was in fact related to the somehow hidden symmetry of the system. That is to say: both the Lagrangian (13) and the constraints (14) of the systems at hand were explicitly independent of the coordinates r_2 and s_α. This property facilitated the reasoning we have applied in our study of the corresponding inverse problems. One possible path to the extension of some of the results in this paper may be the consideration of systems with more general (possibly non-Abelian) symmetry groups. A recent study [10] of the reduction of the invariant inverse problem for invariant Lagrangians may be helpful in that respect.

The methods of the inverse problem have lead us to the Lagrangians for the second associated second-order systems (24). For those systems the q^a-equations were, apart from the coupling with the r_1-equation, all decoupled from each other. It would be of interest to see, for more general systems, how such a form of partial decoupling influences the question of whether or not a regular Lagrangian exists.

In the previous section we have found a new link between the fields of optimal control, where equations are derived from a Hamiltonian, and nonholonomic mechanics, where equations are derived from a Hamiltonian and constraint reaction forces. By combining elements of both derivations, for certain systems one can formulate the mechanics in a form analogous to the treatment of constraints arising from singular Lagrangians that leads to the Dirac theory of constraints [18], which allows for the quantization of constrained systems wherein the constraints typically arise from a singular Lagrangian (see [20] and references therein). Central to the method is the modification of the Hamiltonian to incorporate so-called first and second class constraints.

The method proposed in this paper in a sense provides an analogue to Dirac's theory and allows for the investigation into the quantization of certain nonholonomic systems by similarly modifying the usual Hamiltonian. In attempting to quantize the class of systems we have considered, we can now instead use one of the Hamiltonians found in Proposition 3. We should note that there have already been some attempts to quantize nonholonomic systems [4, 13, 17, 19, 20, 25], and that the results have been mixed, mainly due to the inherent difficulties arising in the quantization procedure, as well as the difficulties in dealing with the system's constraints. However, the present work enables one to treat the constraints more like an initial condition, since, for example, the constraint (43) is really the relation $c_1 + c_2 = 0$, where $p_x = c_1$, and $p_y = c_2$ follows from H in (42) being cyclic in x, y. Such a treatment of the constraints eliminates much of the difficulty arising in attempting to quantize some nonholonomic systems.

As example, consider the knife edge on the plane, in view of (42). We can take the quantum Hamiltonian $\hat{H}$ to be of the form

$$\hat{H} = -\frac{\hbar^2}{2}\left[\frac{\partial}{\partial\phi} - i\frac{\hbar}{2}\left(\cos(\phi)\frac{\partial^2}{\partial x^2} - \sin(\phi)\frac{\partial^2}{\partial y^2}\right)\right]^2, \tag{48}$$

which is a Hermitian operator, and consider the quantum version of the constraint manifold (43) $\hat{p}_x + \hat{p}_y = 0$ (Here $\hat{}$ stands for the quantum operator form under canonical quantization). There have in the literature been essentially two different ways to impose these quantum constraints: *strongly* and *weakly*. One may require that the quantum constraints hold *strongly*, by restricting the set of possible eigenstates of (48) to those which satisfy the quantum operator form of constraint (43). On the other hand, one may only require that the eigenstates $|\psi\rangle$ of (48) satisfy the quantum constraints in mean

$$\langle\psi|\hat{p}_x + \hat{p}_y|\psi\rangle = 0, \tag{49}$$

a weaker condition but arguably a more physically relevant viewpoint also advocated in [17, 19]. In [17] the authors show that (using the example of the vertical rolling disk) the weaker version can be used to recover the classical nonholonomic motion in the semi-classical limit of the quantum dynamics. Details of our application of the methods in this paper to the quantization of nonholonomic systems will be presented in a future publication.

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